Supplementary Information

Ultra-small MgH_2 nanoparticles embedded into an ordered microporous carbon with rapid hydrogen sorption kinetics

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Content:

1) Pore size distribution of pristine ordered microporous carbone CT

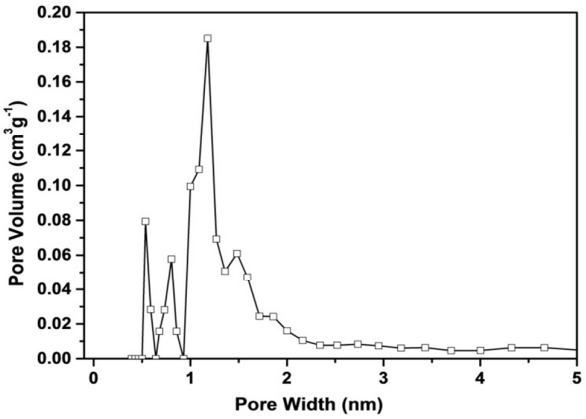

Figure SI-1. Pore size distribution of pristine carbon template CT from zeolite β.

2) Hydrogenation of $MgBu_2$@CT followed by HP-DSC

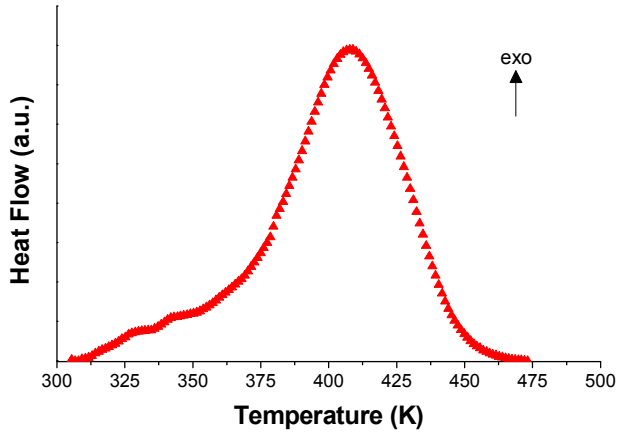

Figure SI-2. HP-DSC curve during hydrogenation reaction: Bu_2Mg@CT + H_2 → MgH_2@CT + $2C_4H_{10}\uparrow$ under 2.5 MPa H_2 with a constant heating rate of 5 $K \cdot min^{-1}$.

3) N_2 sorption measurement at 77 K for all MgH_2@CT composites before (as-synthesized) and after HCl leaching

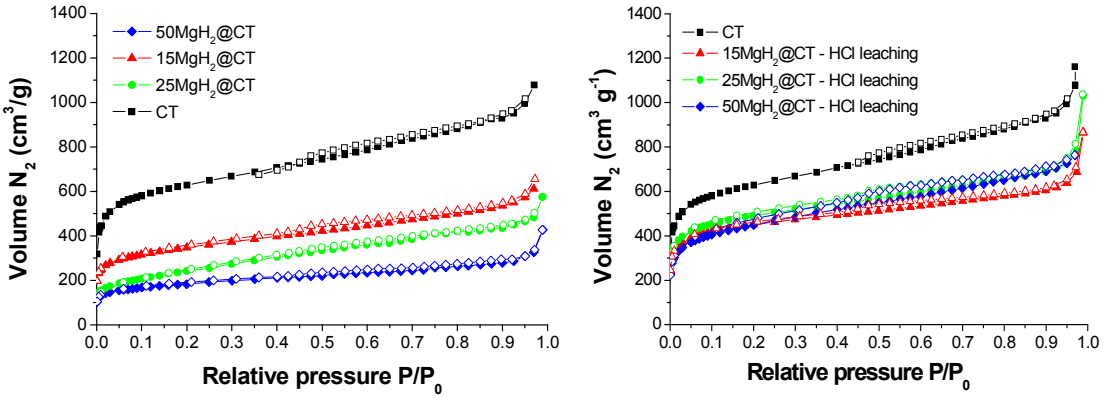

Figure SI-3. N_2 sorption isotherms at 77 K for all MgH_2@CT composites as synthesized (left) and after HCl leaching (right).

4) X-rays diffraction for the pristine CT carbon and the 50MgH_2@CT composite after leaching

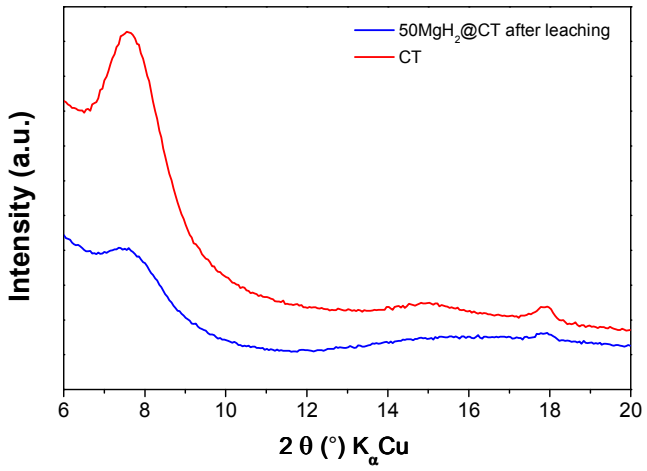

Figure SI-4. X-rays diffraction of the pristine CT and the composite 50MgH_2@CT after leaching.

The X-rays diffractometer used is described in the experimental section. The diffraction peak at 7.5 ° strongly decreases after acid leaching of 50MgH_2@CT as compared to the pristine CT. This indicates a loss of structural ordering by insertion of MgH_2 nanoparticles, in agreement with previous results. [1]

5) Comparative study for the determination of activation energy of desorption of bulk MgH_2

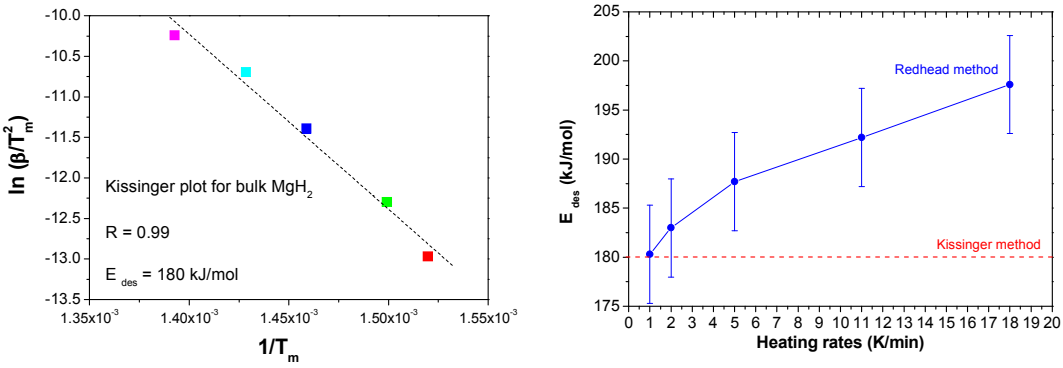

Figure SI-5. Kissinger plot for bulk MgH_2 (left) and the comparison between the activation energies of desorption as calculated from Kissinger and Redhead methods (right).

The E_{des} value calculated by Redhead method [2] for the slowest heating rate (1 $K \cdot min^{-1}$) matches the one determined by Kissinger method suggesting that Redhead equation gives accurate results from our spectra recorded with low heating rates (1-2 $K \cdot min^{-1}$).

6) ^{1}H MAS NMR spectra from the CT, 15MgH_2@CT and 50MgH_2@CT and related deconvolution for 15MgH_2@CT

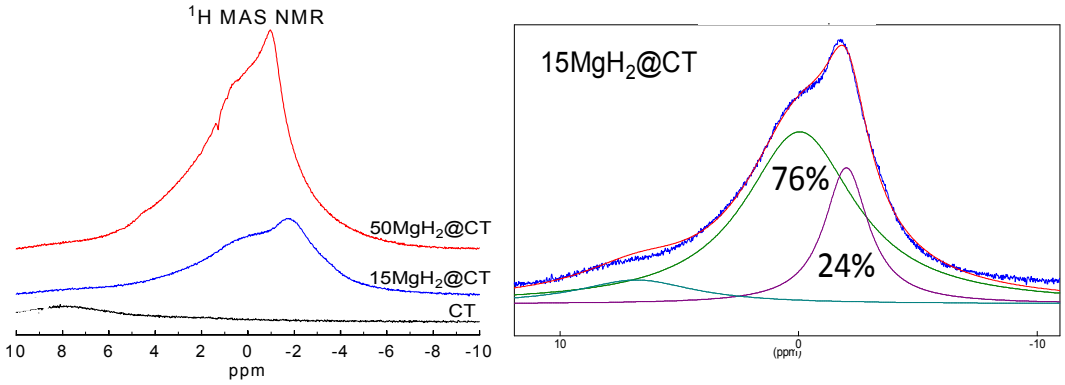

Figure SI-6. ^{1}H MAS NMR spectra from the CT, 15MgH_2@CT and 50MgH_2@CT (left) and related deconvolution for 15MgH_2@CT (right).

References:

[1] C. M. Ghimbeu, C. Zlotea, R. Gadiou, F. Cuevas, E. Leroy, M. Latroche, and C. Vix-Guterl, J. Mater. Chem. **21**, 17765 (2011).

[2] A. Dejong and J. Niemantsverdriet, Surf. Sci. **233**, 355 (1990).